INFORMATION TO USERS

This manuscript has been reproduced from the microfilm master. UMI films the text directly from the original or copy submitted. Thus, some thesis and dissertation copies are in typewriter face, while others may be from any type of computer printer.

The quality of this reproduction is dependent upon the quality of the copy submitted. Broken or indistinct print, colored or poor quality illustrations and photographs, print bleedthrough, substandard margins, and improper alignment can adversely affect reproduction.

In the unlikely event that the author did not send UMI a complete manuscript and there are missing pages, these will be noted. Also, if unauthorized copyright material had to be removed, a note will indicate the deletion.

Oversize materials (e.g., maps, drawings, charts) are reproduced by sectioning the original, beginning at the upper left-hand corner and continuing from left to right in equal sections with small overlaps. Each original is also photographed in one exposure and is included in reduced form at the back of the book.

Photographs included in the original manuscript have been reproduced xerographically in this copy. Higher quality 6" x 9" black and white photographic prints are available for any photographs or illustrations appearing in this copy for an additional charge. Contact UMI directly to order.

UMI

A Bell & Howell Information Company
300 North Zeeb Road, Ann Arbor MI 48106-1346 USA
313/761-4700 800/521-0600

SPECTRAL APPROXIMATION BY THE POLAR TRANSFORMATION

WEI HUA ZHOU

A Thesis

in

The Department

of

Mathematics and Statistics

Presented in Partial Fulfillment of Requirements

for the Degree of Master of Science at

Concordia University

Montreal, Quebec, Canada

April 1997

ABSTRACT

Spectral Approximation by the Polar Transformation

Wei Hua Zhou

Central potentials $V(r)$ are considered which admit the polar representation $V(r) = g(h(r))$, where $h(r) = \mathrm{sgn}(q)r^q$, q is fixed, and g is the polar transformation function. This representation allows the Schrödinger eigenvalues generated by V to be approximated in terms of those generated by the polar potential $h(r)$. In many cases the optimal values $\{q_1, q_2\}$ of the power q can be chosen so that the corresponding polar functions $\{g_1, g_2\}$ have definite and opposite convexity. For such cases, the spectral approximations provide both upper and lower bounds for the entire discrete spectrum. The example of the central potential $V(r) = ar^2 + br^2/(1 + cr^2)$ in R^3 is studied in detail: optimal bounds are determined for a wide range of the potential parameters. The method is applicable, essentially unchanged, for problems in any number of spatial dimensions.

To My Parents

&

Wife and Son

ACKNOWLEDGEMENTS

I am greatly indebted to my supervisor, Dr. R. L. Hall, for his invaluable help and guidance. It would have been impossibe to accomplish this task without his guidance. I feel honoured to be Dr. Hall's graduate student.

I am also grateful to Dr. S. T. Ali, former Graduate Program Director of the Department of Mathematics, Concordia University, for his help and kindness. A road accident had lost me much time, it would have been impossible to have continued my study without his help.

I wish, as well, to thank my friends N. Saad and D. Dalpé, for reading the manuscript. Thanks are also due to all who have helped me in my study and life.

TABLE OF CONTENTS

CHAPTER I

INTRODUCTION

We consider a single particle which moves in an attractive central potential $V(r)$. The number of spatial dimensions is, in principle, arbitrary but, for definiteness of our presentation, we shall usually take it to be *three*. For convenience we assume units in which $\hbar = 2m = 1$. Thus the Hamiltonian H may be written

$$H = -\Delta + V(r). \tag{1.1}$$

The class of potentials we consider comprises those that admit the polar representation

$$V(r) = g(h(r)), \quad h(r) = \mathrm{sgn}(q) r^q, \tag{1.2}$$

where q is a constant and the polar transformation function $g(h)$ is monotone increasing. For definiteness, and to allow broad generality, we shall assume (in *three* dimensions) that $q > -2$, $q \neq 0$. In Section III.1 a detailed analysis of the transformation $g(h)$ is presented. However, the approach can easily accommodate special Hilbert spaces required, for example, by more singular potentials.

Our principal tool is still the "potential envelope method" which, in the particular case of the polar 'envelope basis' $h(r)$, allows us [14] to approximate the eigenvalues by means of the following semi-classical expression

$$E_{nl} \approx E_{nl}^{(A)}(q) = \min_{r>0} \left\{ (\frac{P_{nl}(q)}{r})^2 + V(r) \right\}, \tag{1.3}$$

where the positive numbers $P_{nl}(q)$ are determined [15] (see Section III.1) by the eigenvalues of the pure polar potential $h(r)$. A very important property of the approximate eigenvalues $E_{nl}^{(A)}(q)$ is that they are monotonically increasing functions of q : from (1.3) it is clear that they increase monotonically with P, and it has been proved [15] that the P are monotonic with respect to q (see Section IV.2). The transformation function $g(h)$ does not appear in this expression but it plays a vital rôle in establishing energy *bounds:* if g is convex, we obtain *lower* bounds, and if g is concave, we obtain *upper* bounds. These bounds are valid for all the discrete eigenvalues, and they hold for all values of the parameters in $V(r)$ for which the appropriate convexity condition is satisfied.

Our main example is the perturbed harmonic oscillator

$$V(r) = ar^2 + \frac{br^2}{1+cr^2}, \quad a, b, c > 0, \tag{1.4}$$

This problem has received much attention in the literature [16–31] mostly in *one* spatial dimension. It is the aim of this thesis to complete the investigation started in an earlier paper [1] by formulating the envelope method in such a fashion that it yields both upper and lower energy bounds for a wide range of the potential parameters. The formulas we obtain apply equally well to any number of spatial dimensions. For definiteness, we discuss the general problem in *three* dimensions and present some numerical results for both *one* and *three* dimensions. In Section IV.3 we shall determine the optimal values $\{q_1, q_2\}$ of q (depending on the parameters) which guarantee respectively that $g'' > 0$ and $g'' < 0$ so that, with these values of q, the formula (1.3) yields lower and upper energy bounds.

The potential envelope method was established based on the Min–Max Principle and the Comparison Theorem [2]. In Chapter II we discuss the background of the method. In Chapter III we present a sketch of the theory, and the procedure of the method. The pure polar potential will serve as an introduction to the general geometrical theory.

In Chapter V specific numerical results are presented with the potential parameter values, and the optimal choices for the power q. Our conclusions are presented in Chapter VI.

CHAPTER II

BACKGROUND

II.1 The Minimum–Maximum Principle

Let $\mathcal{H}$ be a complex Hilbert space having the scalar product (ϕ, ψ) and the corresponding norm $\|\psi\| = (\psi, \psi)^{1/2}$. Note that, we shall retain this definition of $\mathcal{H}$ throughout the thesis. Let H be a self–adjoint operator on a domain $\mathcal{D}_H$ dense in $\mathcal{H}$. We shall always assume that H is bounded below and that the lower part of its spectrum consists of a finite or infinite number of discrete eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3 ...$, each having finite multiplicity.

First of all, we give a variational characterization of the discrete spectrum of H. This is the starting point for our discussion of the variational theory of eigenvalues. The following principle, which characterizes the eigenvalues without any reference to the eigenvectors, is often useful in theoretical work.

The Min–Max Principle [2]:

Let D_n denote any n–dimensional subspace of $\mathcal{H}$ contained in $\mathcal{D}_H$ (n=1,2,3,...). We define the *Rayleigh quotient* as

$$R(\psi) = \frac{(H\psi, \psi)}{\|\psi\|^2}, \quad \psi \neq 0. \tag{2.1.1}$$

Let β be the maximum of the *Rayleigh quotient* with $\psi \in D_n$. The β depends, of course, on the choice of D_n and will be denoted by $\beta(D_n)$. Then the eigenvalues of H are characterized by the equation

$$\lambda_n = \min_{D_n} \beta(D_n), \tag{2.1.2}$$

or

$$\lambda_n = \min_{D_n} \max_{\psi \in D_n} \frac{(H\psi, \psi)}{\|\psi\|^2} = \min_{D_n} \max_{\substack{\psi \in D_n, \\ \|\psi\|=1}} (H\psi, \psi). \tag{2.1.3}$$

Remarks: In what follows the restriction $\psi \neq 0$ is always imposed.

a) To find the nth eigenvalue according to this Min–Max principle, one has to proceed as follows: Take the maximum β of the Rayleigh quotient, not on the set of all vectors in $\mathcal{D}_H$ but rather the restricted maximum on an n–dimensional subspace D_n of $\mathcal{H}$ contained in $\mathcal{D}_H$. That is to say, $D_n = \text{Span}\{\psi_1, \psi_2, ..., \psi_n\}$, where $\psi_i \in \mathcal{D}_H$, $i = 1, 2, ..., n$. "min" over "D_n" means that the minimum value is over all possible n–dimensional subspaces D_n so constructed.

b) For a given angular momentum subspace of $\mathcal{L}^2(\mathcal{R}^3)$ labelled by the spherical harmonic $Y_l^m(\theta, \phi)$, where l is fixed, $m = -l, -l+1, ..., l$, the nth eigenvalue E_{nl} of the Schrödinger operator H satisfies

$$E_{nl} = \min_{D_{nl}} \max_{\substack{\psi \in D_{nl} \\ \|\psi\|=1}} (H\psi, \psi), \tag{2.1.4}$$

where $D_{nl} \subset \mathcal{D}_H$ is a finite-dimensional subspace of $\mathcal{H}$ of fixed dimension n ($n = 1, 2, 3, ...$) given by

$$D_{nl} = \text{Span}\{\psi_1, \psi_2, ..., \psi_n\},\ \psi_i \in \mathcal{D}_H,$$

$$\psi_i = u_i(r) Y_l^m(\theta, \phi),\ i = 1, 2, ..., n.$$

II.2 The Comparison Theorem

From the Min–Max principle, there follows an important theorem which in many cases allows comparison to be made between the eigenvalues of two operators. This can have both quantitative and qualitative consequences. Before formulating the theorem, we need the following definition.

Definition:

Let H_1 and H_2 be self–adjoint operators that are bounded below, and $\mathcal{D}_{H_2} \subseteq \mathcal{D}_{H_1}$. Then we say

$$H_1 \leq H_2 \tag{2.2.1}$$

if and only if

$$(H_1\psi, \psi) \leq (H_2\psi, \psi) \tag{2.2.2}$$

for all $\psi \in \mathcal{D}_{H_2}$.

As an immediate consequence of this definition and the Min–Max principle, we have the following theorem.

The Comparison Theorem [2]:

Let H_1 and H_2 be self–adjoint operators that are bounded below, where $H_1 \leq H_2$. If λ_n and μ_n are eigenvalues of H_1 and H_2 respectively, and set out in sequences of increasing magnitude, then

$$\lambda_n \leq \mu_n, \quad n = 1, 2, 3, ... \tag{2.2.3}$$

In the case $(H_1\psi,\psi) < (H_2\psi,\psi)$ for all $\psi \in \mathcal{D}_{H_2}$, it is clear that in (2.2.3) we have a strict inequality, and therefore

$$\lambda_n < \mu_n, \quad n = 1, 2, 3, ... \tag{2.2.4}$$

The principal class of operators we shall look at in this thesis is the *Schrödinger operator* $H = -\Delta + V(r)$ acting on a suitable domain $\mathcal{D}_H$ in $\mathcal{L}^2(\mathcal{R}^3)$. Here $-\Delta$ is the Laplacian kinetic–energy operator, $V(r) = vf(r)$ $(r = |\mathbf{r}|)$, is the potential energy operator, f is the shape of the central potential, and v is a positive coupling constant. If

$$H_1 = -\Delta + V_1(r), \tag{2.2.5}$$

$$H_2 = -\Delta + V_2(r), \tag{2.2.6}$$

with the same boundary conditions and

$$V_1(r) \leq V_2(r) \qquad \text{for all } r > 0, \tag{2.2.7}$$

then the Comparison Theorem provides that

$$\lambda_n \leq \mu_n, \qquad \text{for all } n, \tag{2.2.8}$$

since we have

$$(H_1\psi,\psi) \leq (H_2\psi,\psi) \qquad \text{for all } \psi \in \mathcal{D}_{H_2}. \tag{2.2.9}$$

This result is often called the Comparison Theorem of quantum mechanics [3]. The fact that the order between potentials implies corresponding the order of the eigenvalues is an essential tool for solving many problems of quantum mechanics: it allows us to *bound* the eigenvalues by the use of comparisons with soluble potentials.

Remark:

A central potential [4] is a real-valued function that is a function of $r = |\mathbf{r}|$ alone. In this case, if E is an eigenvalue of $H = -\Delta + V(r)$, then $\{\psi | H\psi = E\psi\}$ is a rotationally invariant subspace of $\mathcal{L}^2(\mathcal{R}^3)$ and is spanned by vectors which may be written

$$\psi(r) = r^{-1}\rho(r)Y_l^m(\theta, \phi), \tag{2.2.10}$$

where Y_l^m are the spherical harmonics and

$$\int_0^\infty |\rho(r)|^2 dr < \infty, \tag{2.2.11}$$

and l is the usual angular momentum quantum number ($l = 0, 1, 2, ...$). If $\psi \in \mathcal{D}_{-\Delta}$, it is bounded and continuous, so $\rho(r)$ is continuous and $\rho(0) = 0$. Moreover , ρ obeys the radial differential equation

$$\left(-\Delta + \frac{l(l+1)}{r^2} + V(r)\right)\rho(r) = E\rho(r). \tag{2.2.12}$$

II.3 Operators: Self–Adjoint and Bounded Below

Definition [5]:

Let H be a linear operator on $\mathcal{H}$, with domain $\mathcal{D}_H$ which is dense in $\mathcal{H}$. Denote by $\mathcal{D}_{H^*}$ the set of all vectors $\phi \in \mathcal{H}$ which are such that for each ϕ there is one and only one vector ϕ^* which satisfies the equation

$$(\phi^*, \psi) = (\phi, H\psi), \quad \text{for all } \psi \in \mathcal{D}_H, \tag{2.3.1}$$

the mapping

$$H^* : \quad \phi \longrightarrow \phi^* \quad \phi \in \mathcal{D}_{H^*}, \tag{2.3.2}$$

is a linear operator, called the *adjoint* of H.

Definition [5]:

The linear operator H acting in $\mathcal{H}$ is *symmetric* if it has an adjoint H^* and $H \subseteq H^*$. A symmetric operator H is called *self–adjoint* if $H^* \subseteq H$, i.e., $H \equiv H^*$.

Here, $H \subseteq H^*$ means that H^* is an extension of H, which defined on $\mathcal{D}_{H^*} \supset \mathcal{D}_H$ coincides with H on $\mathcal{D}_H$ i.e. $H^*\phi = H\phi$ for all $\phi \in \mathcal{D}_H$ *–mutatis mutandis* for $H^* \subseteq H$. Clearly, $H \equiv H^*$ implies $\mathcal{D}_H = \mathcal{D}_{H^*}$.

Self–adjoint operators play a major role in mathematical physics, and in functional analysis. Since the physical interpretation requires that operators which represent measurable physical quantities must be self–adjoint: the eigenvalues (if any) are real and may therefore correspond to the outcomes of physical measurements.

Remarks: It is important to note that [7]

a) The spectrum of a self–adjoint operator is entirely on the real axis.

b) A real scalar multiple of a self–adjoint operator is self–adjoint.

Definition:

A symmetric operator H on $\mathcal{D}_H$ is said to be *bounded below* if there exists a constant k (possibly negative) such that

$$(H\psi, \psi) \geq k\|\psi\|^2 \qquad \text{for all } \psi \in \mathcal{D}_H. \tag{2.3.3}$$

A symmetric operator H on $\mathcal{D}_H$ is *bounded above* if there exists a constant k such that

$$(H\psi, \psi) \leq k\|\psi\|^2 \qquad \text{for all } \psi \in \mathcal{D}_H. \tag{2.3.4}$$

Since the spectral properties of operators on infinite–dimensional spaces are more complicated than on finite–dimensional spaces, some limitations will have to be imposed on the operators under consideration. One obvious difficulty is that the eigenvalues may now extend all the way to $+\infty$ or $-\infty$, if the operator is unbounded. For instance , the kinetic–energy operator $-\Delta = -d^2/dx^2$ on the domain $\mathcal{D}_{-\Delta}$ of function $\phi(x)$ with two continuous derivatives in $0 \leq x \leq 1$, and satisfying $\phi(0) = \phi(1) = 0$ gives rise to eigenvalues $\lambda_n = n^2\pi^2$ (see Remark b below), and clearly $\lambda_n \to +\infty$ as $n \to \infty$.

We can therefore only hope to have a Min–Max principle which works its way up from the low end of the spectrum (that is, starting from λ_1). In our discussion we shall consider only *semi–bounded* operators, that is, operators which are either *bounded below* (as in the example just given, $-\Delta$) or *bounded above* (for instance, the operator $\Delta, \Delta = d^2/dx^2$). In particular, we consider those *bounded below*, since, *mutais mutandis*, we can easily state similar results for operators *bounded above.*

Remarks:

a) The definition for a *bounded* operator H is as follows: There exists a constant $c \geq 0$ such that

$$\|H\psi\| \leq c\|\psi\|, \qquad \text{for all } \psi \in \mathcal{D}_H. \tag{2.3.5}$$

By Schwarz inequality we have

$$|(H\psi, \psi)| \leq \|H\psi\|\|\psi\| \leq c\|\psi\|^2, \tag{2.3.6}$$

$$-c\|\psi\|^2 \leq (H\psi, \psi) \leq c\|\psi\|^2, \tag{2.3.7}$$

so that a *bounded* operator is *bounded above* and *below*.

b) Consider the operator $-\Delta$ in *one* dimension. We can find those values λ_n for which the differential equation

$$-\frac{d^2\phi}{dx^2} = \lambda_n \phi \tag{2.3.8}$$

has non-trivial solutions, satisfying the conditions

$$\phi(0) = \phi(1) = 0. \tag{2.3.9}$$

The general solution of equation (2.3.8) can be written in the form:

$$\phi(x) = C \sin \sqrt{\lambda_n} x + C_1 \cos \sqrt{\lambda_n} x. \tag{2.3.10}$$

The condition $\phi(0) = 0$ gives $C_1 = 0$ and $\phi(x) = C \sin \sqrt{\lambda_n} x$. From the condition $\phi(1) = 0$ we have that $C \sin \sqrt{\lambda_n} = 0$. Here $C \neq 0$ as otherwise we would have only the trivial solution $\phi = 0$. Thus $\sin \sqrt{\lambda_n} = 0$, and we find the eigenvalues

$$\lambda_n = n^2\pi^2, \qquad n = 1, 2, ..., \tag{2.3.11}$$

and eigenfunctions

$$\phi_n(x) = C_n \sin(n\pi x). \tag{2.3.12}$$

The constants C_n are obtained from the normalization condition

$$\|\phi_n\|^2 = C_n^2 \int_0^1 \sin^2(n\pi x)dx = 1,$$

whence $C_n = \sqrt{2}$ and

$$\phi_n(x) = \sqrt{2}\sin(n\pi x). \tag{2.3.13}$$

c) The Schrödinger operators for atoms such as Hydrogen and Helium, also yield self–adjoint, semi–bounded operators of the type described above [5,6].

II.4 Functions: Convexity and Concavity

Definition:

Let $g(h)$ be a continuous function. We define $g(h)$ to be *strictly convex* on an interval of the real line if

$$g(\lambda h_1 + (1-\lambda)h_2) < \lambda g(h_1) + (1-\lambda)g(h_2), \tag{2.4.1}$$

for every pair of distinct points h_1 and h_2 ($h_1 > h_2$) within the interval and for all real λ in $0 < \lambda < 1$.

Geometrically this means that the chord joining any two points on the function always lies above the function between those points. Though this basic analytical definition of convexity is available regardless of whether any derivative of the function exists, if we suppose that $g(h)$ is a smooth function (i.e., C^1–function, which is a continuous function with continuous first derivative), then it follows by calculus that $g(h)$ is *strictly convex* if and only if

$$g(h_1) - g(h_2) - (h_1 - h_2)g'(h_2) > 0 \tag{2.4.2}$$

for every pair of distinct points h_1 and h_2 within the interval. The geometrical interpretation is that the function lies above its tangent line at every point except at the point of contact of the tangent line. This is illustrated in Fig.2.4(a) for a C^1–function. By interchanging h_1 and h_2 in (2.4.2) we have

$$g(h_2) - g(h_1) - (h_2 - h_1)g'(h_1) > 0, \tag{2.4.3}$$

and adding the two results we get

$$(h_1 - h_2)[g'(h_1) - g'(h_2)] > 0, \tag{2.4.4}$$

i.e., the slope of a smooth strictly convex function is monotonically increasing.

Weakly convex is defined by writing $\geq$ in these inequalities so that equality can hold for some distinct pairs of points, thus permitting straight line segments (Fig.2.4(b)). Convexity without an adjective often means weak, but can mean strict, depending on the context.

A *concave* function is a convex function turned upside down, so that the foregoing inequalities are reversed. The C^1–function never rises above its tangent line at any point. In the format of (2.4.2) we can define $g(h)$ to be *strictly concave* if

$$g(h_1) - g(h_2) - (h_1 - h_2)g'(h_1) > 0 \qquad (2.4.5)$$

for every pair of distinct points, the derivate now being evaluated at the opposite end of the interval compared to (2.4.1) (Fig.2.4(c)).
A C^2–function is a continuous function with continuous first and second derivatives. If $g(h)$ is a C^2–function, integration by parts shows that

$$\int_{h_2}^{h_1} (h_1 - h)g''(h)dh = g(h_1) - g(h_2) - (h_1 - h_2)g'(h_2), \qquad (2.4.6)$$

and

$$\int_{h_2}^{h_1} (h_2 - h)g''(h)dh = g(h_1) - g(h_2) - (h_1 - h_2)g'(h_1). \qquad (2.4.7)$$

From (2.4.2), (2.4.6) ((2.4.5), (2.4.7)) we see that a necessary and sufficient condition for $g(h)$ to be *strictly convex* (*concave*) is that

$g''(h) > 0$ ($g''(h) < 0$) everywhere. A necessary and sufficient condition for *weak convexity* (*weak concavity*) is $g''(h) \geq 0$ ($g''(h) \leq 0$) at every point.

If we take a nonlinear change $h = h(r)$ of the independent variable r, for the function $V(r) = g(h) = g(h(r))$ we have $dV/dr = g'dh/dr$, and

$$\frac{d^2V}{dr^2} = \frac{d^2h}{dr^2}g' + (\frac{dh}{dr})^2 g'', \tag{2.4.8}$$

by the chain rule. Clearly, the first term on the right can cause the sign of the curvature of $V(r)$ to change even if g'' has constant sign. Fortunately, the approximation theory we develop only requires definite convexity of $g(h)$, where $g(h)$ is a smooth increasing transformation of h, and $g(h(r)) = V(r)$.

Remarks: It is noteworthy that concave functions g have the following properties [6]:

a) For $h > 0$, $g(h)$ is concave if and only if $h\,g(1/h)$ is concave.

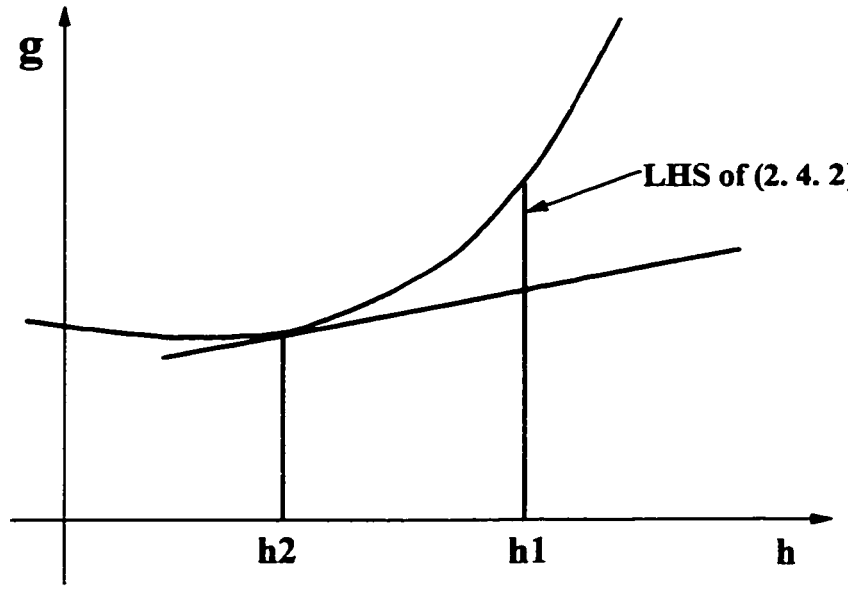
b) If $g > 0$ and $1/g$ is concave, then g is convex.

c) If the functions $g_i(h)$ are concave and $\alpha_i \geq 0$, then $\Sigma_i \alpha_i\, g_i(h)$ is concave ($i = 1, 2, ...$).

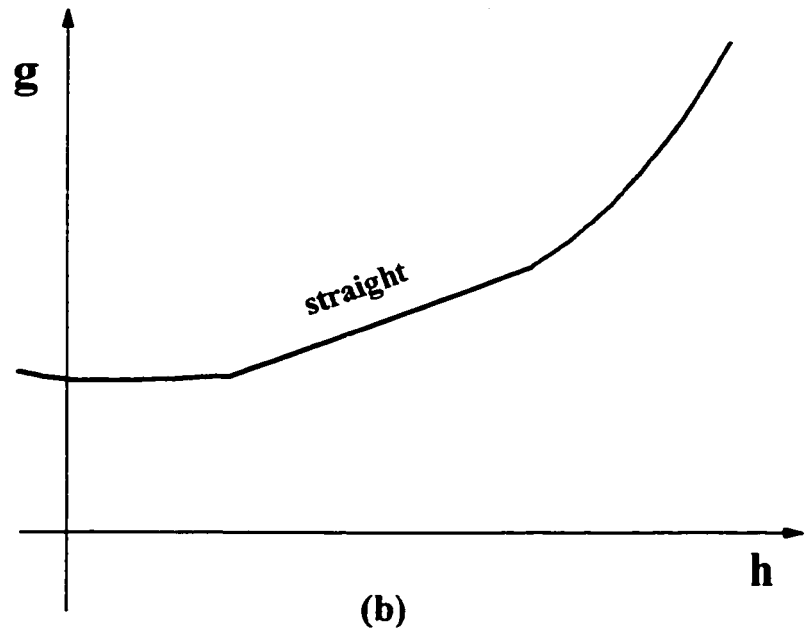
d) If $g_i(h)$ are concave, then $\inf_i\, g_i(h)$ is concave (i=1,2,...).

e) If g_i are concave ($i = 1, 2$), and $g_1' \geq 0$, then $g_1 \circ g_2$ is concave.

Figures 2.4(a) and 2.4(b)

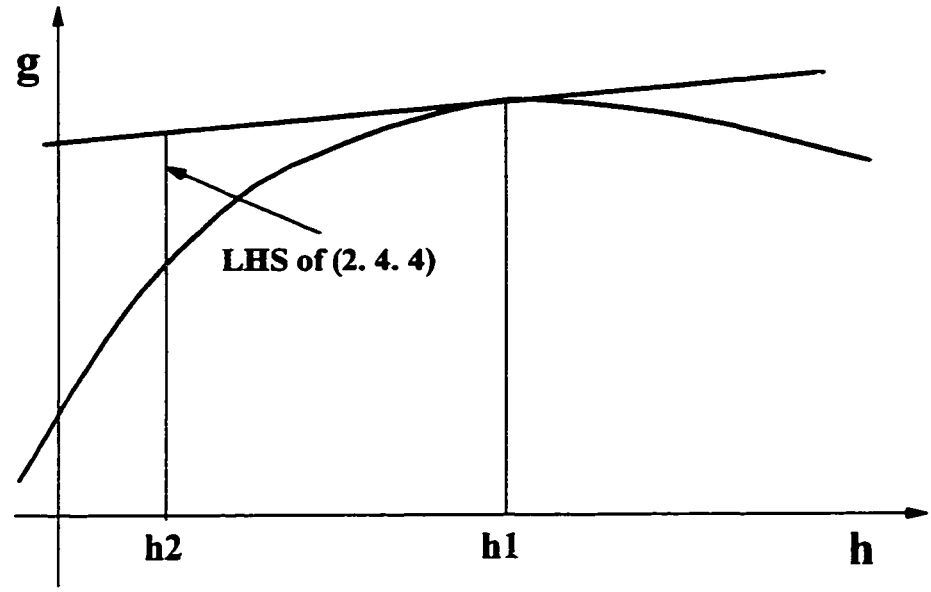


(a)



(b)

Figure 2.4(c)



(c)

CHAPTER III

THE POTENTIAL ENVELOPE METHOD

III.1 The Theory

The method of potential envelope was established by Hall [1]. An essential feature of Hall's approach to spectral geometry is the reformulation of the standard Min–Max characterization of discrete Schrödinger eigenvalues in terms of *mean kinetic energies.*
This method makes use of the Comparison Theorem based on the Min–Max principle and provides approximate analytical expressions for the eigenvalues of Hamiltonians whose potential part $V(r)$ can be presented as a smooth transformation $V(r) = g(h(r))$ of a potential $h(r)$ corresponding to a soluble problem. These simple formulas, for lower and upper bounds, have been shown to give good estimates for the spectra of a number of Hamiltonians, including those with linear combinations of different potentials [9–12]. Some refined inequalities for energy levels have also been derived [13].

We now present a summary of this theory as a basis for understanding the present work. All of the necessary potential–envelope formalism may be found in greater detail in the cited references [1,10,11,14].

Suppose that we can solve the Schrödinger equation

$$\big(-\Delta + vh(r)\big)\psi(r) = \mathcal{E}_{nl}(v)\psi(r), \tag{3.1.1}$$

for the discrete eigenvalues $\mathcal{E}_{nl}(v)$ of the potential $h(r)$, where h is the shape of a central potential. The trajectory function $\mathcal{E}_{nl}(v)$ generates an energy trajectory $(v, \mathcal{E}_{nl}(v))$, $v > 0$, which describes how the eigenvalue depends on the coupling constant: this functional dependence

will be important later; if necessary, the trajectories may have to be defined for $v \geq v_{nl}$ sufficiently large to guarantee the existence of the corresponding eigenvalue. The trajectory functions satisfy

$$\mathcal{E}_{nl}(v) \leq \mathcal{E}_{n'l}(v) \quad (1 \leq n < n'). \tag{3.1.2}$$

The quantum number n counts the eigenvalues in each angular momentum subspace: eigenvalues so labelled have degeneracy exactly equal to $(2l+1)$.

We wish to estimate the eigenvalues when the potential is changed to $V(r)$, under a smooth increasing transformation $g(h(r)), V(r) = g(h(r))$, where g has definite convexity, either convex or concave. That is to say, $g' > 0$ and either $g'' > 0$ or $g'' < 0$. We summarize this situation by the relation

$$-\Delta + vh(r) \longrightarrow \mathcal{E}_{nl}(v), \tag{3.1.3}$$

$$-\Delta + V(r) \longrightarrow E_{nl}, \tag{3.1.4}$$

where the graph $(v, \mathcal{E}_{nl}(v))$ is the exact energy trajectory of $-\Delta + v\,h(r)$ with respect to h.

We now present a brief argument leading to

$$E_{nl} \approx \min_{r>0} \left\{ K_{nl}^{(h)}(r) + V(r) \right\} \tag{3.1.5}$$

where

$$V(r) = g(h(r)), \quad K_{nl}^{(h)}(r) = \mathcal{E}_{nl}(v) - v\,\mathcal{E}'_{nl}(v), \quad h(r) = \mathcal{E}'_{nl}(v), \tag{3.1.6}$$

and, $\approx = \leq$ if g is concave and $\approx = \geq$ if g is convex, which is the key result used in this thesis. This formulation of the potential envelope

method is actually interesting for it tells us (approximately) how the eigenvalues E_{nl} derived from the potential $V(r) = g(h(r))$ depend on the energy trajectories $\mathcal{E}_{nl}(v)$ corresponding to the potential $h(r)$.
For definiteness, we suppose that g is concave so that $g'' < 0$ everywhere in $\mathcal{D}_g$. Because of the concavity of g, we know that the tangent lines to g (as a function of h) all lie above g except at the point of contact, and we can therefore find by calculus that

$$g\big(h(r)\big) \leq A + vh(r), \tag{3.1.7}$$

where

$$A = g\big(h(t)\big) - h(t)g'\big(h(t)\big), \quad v = g'\big(h(t)\big), \quad t \in (0, \infty) \tag{3.1.8}$$

and $h(t)$ is the point of contact of $V(r)$ with its tangent potential

$$V^{(t)}(r) = A(t) + v(t)h(r). \tag{3.1.9}$$

Since the operators we consider are self–adjoint and bounded below, now we can employ the Comparison Theorem of quantum mechanics which tells us that the potential inequality (3.1.7),
i.e. $g\big(h(r)\big) \leq A + vh(r)$, implies the spectral inequality

$$E_{nl} \leq A(t) + \mathcal{E}_{nl}\big(v(t)\big), \tag{3.1.10}$$

that is

$$E_{nl} \leq g(h) - hg'(h) + \mathcal{E}_{nl}\big(g'(h)\big), \tag{3.1.11}$$

where $h = h(t)$.
We minimize the right–hand side of the inequality (3.1.11) with respect to the variable h, since the upper bound is a function of h.

The necessary condition for the minimum is obtained by differentation with respect to h and cancellation of the factor $g''(h) < 0$ (by hypothesis, g is concave). This yields the critical point

$$h = \mathcal{E}'_{nl}(v), \quad v = g'(h). \tag{3.1.12}$$

In view of (3.1.11), (3.1.12) and the known [14] concavity of trajectory functions like $\mathcal{E}_{nl}$, we can reformulate the expression (3.1.11) for the best upper bound by a Legendre transformation [8] as follows:

$$E_{nl} \leq \min_{r>0} \left\{ K_{nl}^{(h)}(r) + V(r) \right\}, \tag{3.1.13}$$

where

$$\begin{aligned} V(r) &= g\big(h(r)\big), \\ K_{nl}^{(h)}(r) &= \mathcal{E}_{nl}(v) - v\,\mathcal{E}'_{nl}(v), \quad h(r) = \mathcal{E}'_{nl}(v). \end{aligned} \tag{3.1.14}$$

The K–functions $K_{nl}^{(h)}(r)$ (relative to h) are well defined by (3.1.14) because $\mathcal{E}_{nl}(v)$ is concave so that $\mathcal{E}'_{nl}(v)$ is monotone and is invertible; they are positive definite and represent *mean kinetic energies* in the envelope approximation. Note that we have used the original variable r in place of the parameter t: in the energy picture there will be no confusion.

What we have in (3.1.13) is a semi–classical approximation which is valid whenever the potential $V(r)$ is a concave transformation $g(h(r))$ of the potential $h(r)$; if the transformation g is convex, then the inequalities are reversed and one obtains lower bounds–i.e.

$$E_{nl} \geq \min_{r>0} \left\{ K_{nl}^{(h)}(r) + V(r) \right\}. \tag{3.1.15}$$

If the potential $V(r)$ depends on various parameters, then the dependence of the energies on these parameters is automatically given by the approximation (3.1.5). A more general formulation of this geometrical theory described in Hall's paper [11], which allows also for sums of soluble potential terms.

For our specific application in this thesis we now consider a smooth transformation g of the pure polar potential $h(r)$,

$$h(r) = \mathrm{sgn}(q) r^q, \quad q > -2, \quad q \neq 0, \tag{3.1.16}$$

which we shall need in Chapter IV.

Here the sign factor $\mathrm{sgn}(q)$ is included to guarantee that the potential is attractive when $q < 0$, that is to say, so that $h'(r) > 0$. For most physical situations the restriction $q \geq -1$ is appropriate, but from a mathematical point of view [4] we can allow $q > -2$. We have (a proof is given in Remark (b) below):

$$-\Delta + v\mathrm{sgn}(q) r^q \longrightarrow \mathcal{E}_{nl}^{(q)}(v) = v^{2/(q+2)} \mathcal{E}_{nl}^{(q)}(1), \tag{3.1.17}$$

where the $\mathcal{E}_{nl}^{(q)}(v)$ are the $\{n, l\}$ eigenvalues of $H = -\Delta + v\mathrm{sgn}(q) r^q$, $l = 0, 1, 2, 3, ...$, is the usual angular momentum quantum number, and $n = 1, 2, 3, ...$, is a radial quantum number which enumerates the discrete eigenvalues in each angular momentum subspace, that is

$$\mathcal{E}_{nl}^{(q)}(v) \leq \mathcal{E}_{n'l}^{(q)}(v), \quad 1 \leq n < n'. \tag{3.1.18}$$

For $q > -2$, $q \neq 0$, all these discrete eigenvalues exist [3].

From (3.1.6) and (3.1.17), we find that

$$K_{nl}^{(h)}(r) = \left(P_{nl}(q)/r\right)^2, \tag{3.1.19}$$

where

$$P_{nl}(q) = |\mathcal{E}_{nl}^{(q)}(1)|^{(2+q)/2q}\Big[\frac{2}{2+q}\Big]^{1/q}\Big[\frac{|q|}{2+q}\Big]^{1/2}, \quad q > -2, \quad q \neq 0. \tag{3.1.20}$$

Consequently, (3.1.5) becomes:

$$E_{nl} \approx E_{nl}^{(A)}(q) = \min_{r>0}\Big\{\Big(\frac{P_{nl}(q)}{r}\Big)^2 + V(r)\Big\}, \tag{3.1.21}$$

where

$$V(r) = g\big(h(r)\big), \quad h(r) = \mathrm{sgn}(q)r^q,$$

and g has definite convexity,

$$\approx = \leq \qquad \text{if } g \text{ is concave,}$$

$$\approx = \geq \qquad \text{if } g \text{ is convex.}$$

By rearranging (3.1.20) we obtain the defining expression for the $\mathcal{E}_{nl}^{(q)}(1)$, that is

$$\mathcal{E}_{nl}^{(q)}(1) = \mathrm{sgn}(q)\eta(q)\,[P_{nl}(q)]^{2q/(2+q)}, \quad q > -2, \quad q \neq 0, \tag{3.1.22}$$

where the function $\eta(q)$ is defined by

$$\eta(q) = \Big[\frac{q}{2} + 1\Big]\Big|\frac{2}{q}\Big|^{\frac{q}{(q+2)}}, \quad q \neq 0; \quad \eta(0) = 1. \tag{3.1.23}$$

A useful interpolation formula is provided [15] by

$$P_{nl}(q) = \Big[(n+l)^\alpha + \frac{q+1}{3}\big[(2n+l-\frac{1}{2})^\alpha - (n+l)^\alpha\big]\Big]^{\frac{1}{\alpha}}, \quad \alpha = 3.2397, \tag{3.1.24}$$

which is exact for $q = -1, 2$, and for $\mathcal{E}_{10}^{(1)}(1)$.

$P_{nl}(q)$ is smoother, less complicated, and easier to approximate than $\mathcal{E}_{nl}^{(q)}(1)$ [15]. The approximate values for $P_{nl}(q)$ given by (3.1.24) yield the pure polar eigenvalues (3.1.22) to within 0.8% (usually much less) for $n, l < 5$, and $-0.5 \leq q \leq 2.5$. In the next section we shall see that the functions $P_{nl}(q)$ behave 'nicely' as functions of q. In particular, they are monotone increasing.

Remarks:

a) The method of potential envelopes is employed to derive a complementary energy–bound formula (3.1.5) valid for all the discrete eigenvalues. The index n of E_{nl} has been chosen to start at $n = 1$.

b) Here we prove the relation

$$\mathcal{E}_{nl}^{(q)}(v) = v^{2/(q+2)}\mathcal{E}_{nl}^{(q)}(1).$$

Suppose $H = -\Delta + v\,\mathrm{sgn}(q)\, r^{(q)}$, and $\mathcal{E}_{nl}^{(q)}(v)$ are discrete eigenvalues of H, i.e.

$$H\,\psi(r) = \mathcal{E}_{nl}^{(q)}(v)\psi(r). \tag{3.1.25}$$

Now, let $\gamma = r/\sigma, (\sigma > 0), \phi(\gamma) = \psi(r)$, then

$$\frac{d^2\phi}{dr^2} = \frac{d^2\phi}{d\gamma^2}\,\frac{1}{\sigma^2}, \tag{3.1.26}$$

and,

$$\Big[-\frac{1}{\sigma^2}\Delta + v\sigma^q \mathrm{sgn}(q)\,\gamma^q\Big]\phi = \mathcal{E}_{nl}^{(q)}(v)\phi, \tag{3.1.27}$$

i.e.

$$\Big[-\Delta + v\sigma^{q+2}\mathrm{sgn}(q)\gamma^q\Big]\phi = \sigma^2\mathcal{E}_{nl}^{(q)}(v)\phi. \tag{3.1.28}$$

If we take $\sigma^{q+2}v = 1$, then $\sigma^2 = v^{-\frac{2}{q+2}}$, and

$$\Big[-\Delta + \mathrm{sgn}(q)\gamma^q \Big]\phi = v^{-\frac{2}{q+2}} \mathcal{E}_{nl}^{(q)}(v)\phi, \tag{3.1.29}$$

or equivalently

$$\Big[-\Delta + \mathrm{sgn}(q)\gamma^q \Big]\phi = \mathcal{E}_{nl}^{(q)}(1)\phi. \tag{3.1.30}$$

Hence, we have $\mathcal{E}_{nl}^{(q)}(v) = v^{2/(q+2)}\mathcal{E}_{nl}^{(q)}(1)$.

c) Whenever the trajectory function $\mathcal{E}_{kl}(v)$ is known for the kth excited state of the base problem $-\Delta + v\,h(r)$, the corresponding energy bound formula yields a bound on the kth eigenvalue E_{kl} of the transformed problem $-\Delta + V(r)$, since the Comparison Theorem applies to each eigenvalue separately.

d) It is of interest to note that the transformation function g does not itself appear in (3.1.5), g is only used to establish the energy bounds by its definite convexity.

e) It is easy to remember "$\approx = \leq$ if g is concave, and $\approx = \geq$ if g is convex" because, for example, if g is concave, then the tangents to $V = g(h)$ lie above V, and we therefore obtain upper bounds; similarly it is clear that we get lower bounds in the convex case.

f) If the convexity of g varies, we can still perform the minimization in (3.1.5) which gives us a critical point $\hat{r}$. We can then determine the convexity of $g(\hat{h})$ at $\hat{h} = h(\hat{r})$, and see if the tangential approximation $V^{(t)}(r) = g'(\hat{h})\,(h(r) - \hat{h}) + g(\hat{h})$ lies entirely on one side of $V(r)$. If these conditions are met, then we can again be sure that E_{nl} is an upper or a lower bound. Unfortunately, if these conditions are not met, we cannot tell whether the approximations are upper or lower bounds.

III.2 The Procedure

A principal application of potential envelope theory is to exploit exact solutions of the Schrödinger equation to approximate solutions of intractable problems. It follows from the discussion in Section III.1 that the potential envelope method should be applied with great care to the choice of transformation function $g(h)$. In the usual procedure, the basic guidelines are: the first thing we do is to choose the basis potential $h(r)$ carefully such that $H = -\Delta + vh(r)$ corresponds to an exactly soluble problem. Then we must choose the convex or concave transformation $g(h)$ of h which generates the new operator $H = -\Delta + g(h)$, where $g(h(r)) = V(r)$, whose eigenvalue we seek. In order to be sure about energy bounds, we must study the transformation function g to determine its convexity. Once this analysis is completed, the function g can be ignored since the eigenvalue approximations are given by (3.1.5) and no longer involve g.

We should mention at this point that two different choices can be made for $V(r)$. Ideally one seeks a dual representation for the potential $V(r)$ in the form

$$V(r) = g_1\big(h_1(r)\big) = g_2\big(h_2(r)\big), \tag{3.2.1}$$

where g_1 is convex, leading to a lower bound, and g_2 is concave, leading to an upper bound, without the use of a trial function. For example, for the pure linear potential we can write

$$r = -(-r^{-1})^{-1} = (r^2)^{1/2}, \tag{3.2.2}$$

where

$$r = g_1\big(h_1(r)\big) = -\big(h_1(r)\big)^{-1}, \quad h_1(r) = -r^{-1}, \tag{3.2.3}$$

and

$$r = g_2(h_2(r)) = \big(h_2(r)\big)^{1/2}, \quad h_2(r) = r^2. \tag{3.2.4}$$

Clearly, $g_1'' > 0$, for all $h_1(r) < 0$; $g_2'' < 0$ for all $h_2(r) > 0$. Hence g_1 is convex and g_2 is concave.

Naturally we look for basis potentials $h_1(r)$ and $h_2(r)$ that closely resemble $V(r)$, thus leading to good eigenvalue approximations. The corresponding K–function $K_{nl}^{(h)}$ (relative to h) are as follows,

$$-\Delta + vh(r) \longrightarrow \mathcal{E}_{nl}(v), \tag{3.2.5}$$

$$K_{nl}^{(h)}(r) = \mathcal{E}_{nl}(v) - v\mathcal{E}'_{nl}(v),\ h(r) = \mathcal{E}'_{nl}(v), \tag{3.2.6}$$

Since the basis potentials, by hypothesis, yield soluble eigenproblems they have usually been discussed in some earlier published work. For example, among the pure polar potentials, the well-known examples of the Coulomb potential and the harmonic oscillator are given [14] respectively by

$$\begin{aligned} h(r) = -r^{-1} &\to \mathcal{E}_{nl}^{(-1)}(v) = -\frac{v^2}{4(n+l)^2} \\ &\to K_{nl}^{(h)}(r) \ = \left(\frac{n+l}{r}\right)^2, \end{aligned} \tag{3.2.7}$$

$$\begin{aligned} h(r) = r^2 &\to \mathcal{E}_{nl}^{(2)}(v) = v^{\frac{1}{2}}(4n + 2l - 1) \\ &\to K_{nl}^{(h)}(r) = \Big(\frac{2n + l - \frac{1}{2}}{r}\Big)^2. \end{aligned} \tag{3.2.8}$$

Meanwhile, in one spatial dimension we have, for the harmonic oscillator

$$h(x) = x^2 \longrightarrow K_n^{(h)}(x) = (n - 1/2)^2/x^2, \tag{3.2.9}$$

and for the sech-squared potential [14]

$$h(x) = -\text{sech}^2(x) \longrightarrow K_n^{(h)}(x) = \frac{1}{\sinh^2 2x} + \frac{n(n-1)}{\sinh^2 x}, \qquad (3.2.10)$$

where $n = 1, 2, 3, ...$

We now look at the question of critical points in (3.1.5). Usually they are given analytically by the equation $E'(r) = 0$, where $E(r) = K_{nl}^{(h)}(r) + V(r), (r > 0)$, and the prime denotes differentiation with respect the variable r. We may use any root–finding method to solve the equation for $\hat{r}$; then substitute this $\hat{r}$ in $E(r)$ to yield the eigenvalue bound $E(\hat{r})$. The question whether $E(\hat{r})$ is an upper or lower bound depends on the convexity of $g(h)$. Sometimes the bounds will turn out to be rather weak. It may then be possible to improve the accuracy by optimizing the bounds over classes of basis potentials. For example, if we take the pure polar potential $h(r) = \text{sgn}(q)r^q$ (3.1.16) as basis potential for $V(r)$, a proper treatment would necessarily involve the choice of an ideal value of the power q, our policy would be to keep $V(r)$ fixed, and to adjust $h(r)$, by varying q in order to choose the optimal q for each bound, whilst maintaining the appropriate convexity of g. We believe that the accuracy of our results may be improved even further with a better choice of q. In Section IV.3 we will see this effect.

Remark:

All our general arguments apply in the same fashion for problems in one dimension. (or, indeed, to problems in any number of spatial dimensions). In *one* dimension, the power–laws $f(x) = |x|^q$ for $q < 0$ require a special vanishing condition on the wave function at $x = 0$

and consequently we cannot use families of such functions to model a nonsingular potential because the problems have different Hilbert spaces. Thus, for nonsingular potentials, hyperbolic envelopes ($q = -1$) are not generally useful in *one* dimension.

CHAPTER IV

A PERTURBED HARMONIC OSCILLATOR

IV.1 The Potential $V(r) = ar^2 + br^2/(1+cr^2)$

Since 1977 there has been much interest in the quantum potential

$$V(r) = ar^2 + \frac{br^2}{1+cr^2}, \quad a,b,c > 0, \tag{4.1.1}$$

from both the physical and mathematical points of view, and a variety of techniques have been employed to obtain approximate eigenvalues and eigenvalue bounds [16–31]. One of the earliest studies was by Mitra [16] who calculated the ground state and first two excited state energies (in *one* dimension) by using the Ritz variational method in combination with the Givens–Householder matrix eigenvalue algorithm. The physical interest in this potential arises in several areas, as summarized by Mitra: in laser theory it arises out of the Fokker–Planck equation for a single–mode laser; in field theory it provides a simple zero–dimensional model possessing a nonlinear Lagrangian. Unfortunately, little information is available in the context of *three*–dimensional quantum systems with this potential.

In 1980, when Hall first introduced "The Method of Potential Envelope", he considered the potential (4.1.1) as an illustration of the theory [1]. The results were obtained by an application of the simple universal formula which gives F_U and F_L (the subscripts refer to "upper" and "lower" bounds) directly in terms of the potential shape f. In this paper [1] the energy of an N–boson problem was related to the

energy of a *one*–body (reduced *two*–body) problem and the envelope method was applied to the latter. We reprint the figures Fig.4.1(a) and Fig.4.1(b) which show us the early results of Hall [1].

It is the aim of this thesis to complete the investigation started in the earlier work by formulating the envelope method in such a fashion that it yields new results for a wide range of potential parameters, for both upper and lower energy bounds.

Figures and Figure Caption

Fig.4.1(a)

Trajectory bounds for the perturbed harmonic oscillator with shape $f(r) = [r^2 + r^2/(1+r^2)]$ in three dimensions. The points $\odot$ are the energies of the first excited state of the *two*-body problem in *one* dimension obtained by Mitra [16] and Kaushal [18]; for $v^{1/2} = 1$ and $v^{1/2} = 2$, these values differ significantly and the upper points are those of Mitra. With $(a = b = c = 1, v = 1)$ and $(a = b = 1, c = 0.5, v = 4)$, for example, the sequences of $(F_L(v), K, M, F_U(v))$ for E_{10} are, respectively, (3.220. 3.305, 3.507, 3.589) and (7.053, 6.918, 7.428, 7.637). K: obtained by Kaushal, M: obtained by Mitra.

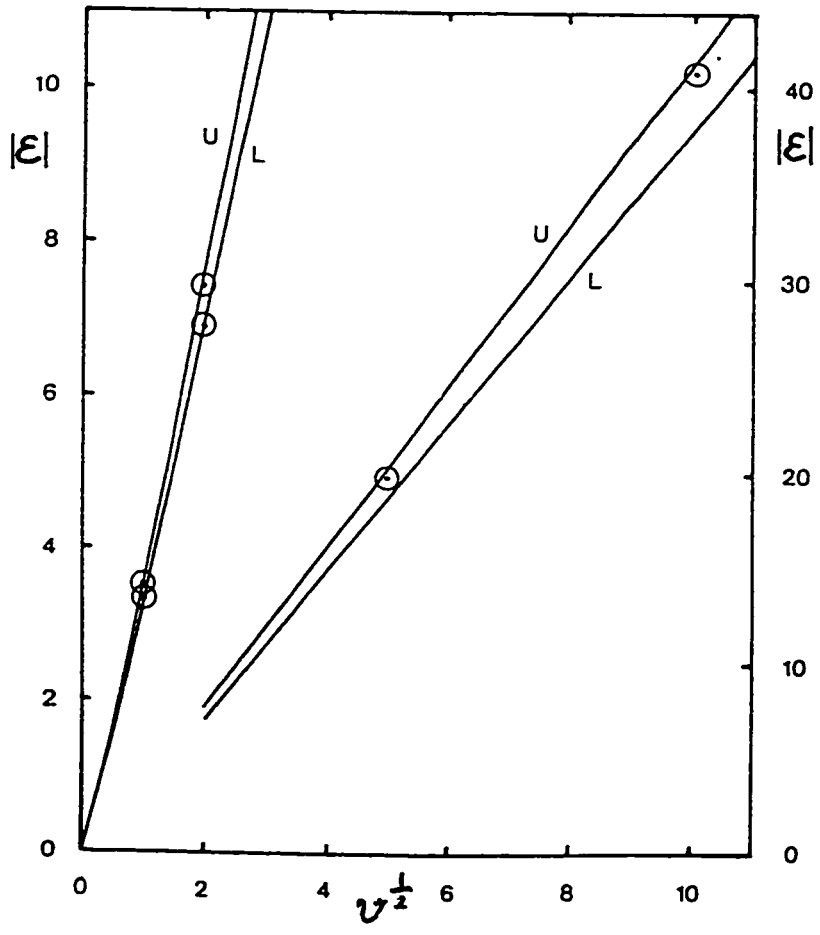
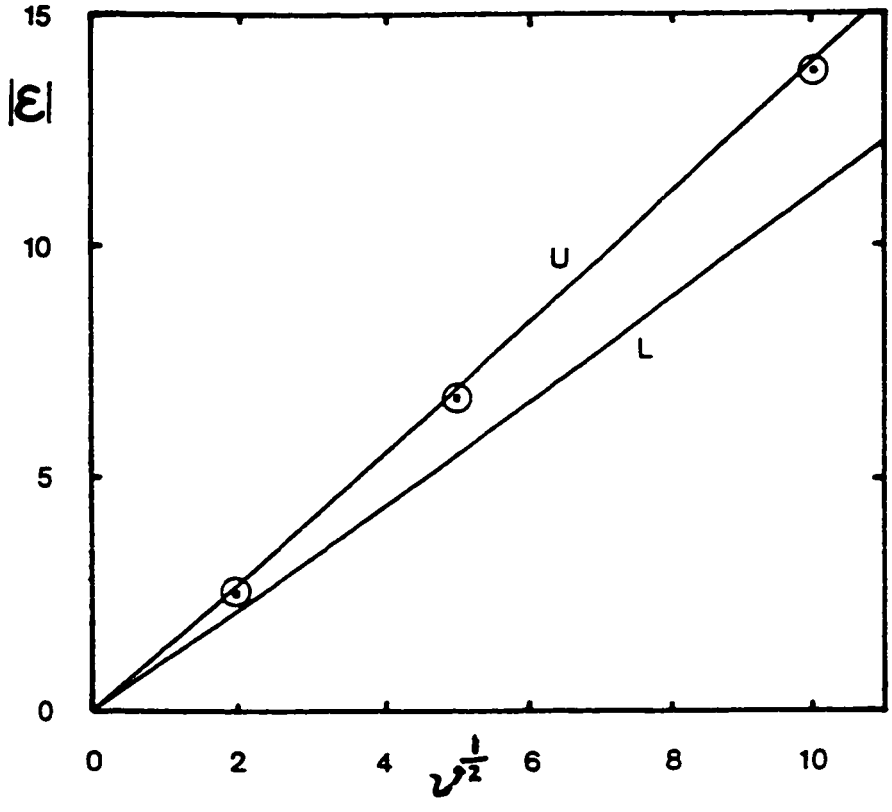


Fig.4.1(b)

Trajectory bounds for the perturbed harmonic oscillator with shape $f(x) = [x^2 + x^2/(1+x^2)]$ in *one* dimension. The points $\odot$ are the energies of the *two*-body problem obtained by Mitra [16] and Kaushal [18].



IV.2 The Functions $P_{nl}(q)$ and $E_{nl}^{(A)}(q)$

In Section III.1 we introduced a special function $P_{nl}(q)$,

$$P_{nl}(q) = |\mathcal{E}_{nl}^{(q)}|^{(2+q)/2q} \left[\frac{2}{2+q}\right]^{1/q} \left[\frac{|q|}{2+q}\right]^{1/2}, \; q > -2, \; q \neq 0, \quad (4.2.1)$$

where

$$\mathcal{E}_{nl}^{(q)} = \mathcal{E}_{nl}^{(q)}(1), \quad (4.2.2)$$

and $\mathcal{E}_{nl}^{(q)}(1)$ is the $\{n, l\}$ eigenvalue of $H = -\Delta + \text{sgn}(q)r^q$.
It has been proved [15] that the $P_{nl}(q)$ are monotone increasing in q. Consequently, approximations $E_{nl}^{(A)}(q)$ deduced from (3.1.5), that is

$$E_{nl}^{(A)}(q) = \min_{r>0} \left\{ \left(\frac{P_{nl}(q)}{r} \right)^2 + V(r) \right\}, \quad (4.2.3)$$

are also monotone increasing in q. This is a very important property of the approximate eigenvalues $E_{nl}^{(A)}(q)$ based on the representation $V(r) = g(\text{sgn}(q)r^q)$. The proof is as follows [15].

First, we write one pure polar potential $\text{sgn}(p)r^p$ as a function g of another $\text{sgn}(q)r^q$:

$$\text{sgn}(p)r^p = g\big(\text{sgn}(q)r^q\big) = g(h), \quad h = \text{sgn}(q)r^q \quad pq \neq 0, \quad (4.2.4)$$

where, for each fixed p and q, $p \neq q$, g is either convex or concave. We have

$$g(h) = \text{sgn}(p)\big(h\,\text{sgn}(q)\big)^{p/q}, \quad (4.2.5)$$

and $h\,\text{sgn}(q) = r^q > 0$. Consequently, we find

$$g'(h) = |p/q|\big(h\,\text{sgn}(q)\big)^{(p/q-1)} > 0, \quad (4.2.6)$$

and

$$g''(h) = \frac{|p|}{q^2}(p-q)\big(h\,\mathrm{sgn}(q)\big)^{(p/q-2)}. \tag{4.2.7}$$

Clearly, if $p > q$, then $g'' > 0$, the function g is strictly convex; if $p < q$, then $g'' < 0$, the function g is strictly concave.

Having established definite convexity properties for the transformation g, we can now exploit the variational implications, by using *kinetic potentials* $\bar{h}_{nl}(s)$. Note that the $\bar{h}_{nl}(s)$ are relative to the potential $h(r)$. This name is a contraction of the more explanatory term *minimum mean isokinetic potential* [11].

We have the following general parametric form for $\bar{h}_{nl}(s)$ in terms of the trajectory function $\mathcal{E}_{nl}(v)$:

$$s = \mathcal{E}_{nl}(v) - v\mathcal{E}'_{nl}(v), \quad \bar{h}_{nl}(s) = \mathcal{E}'_{nl}(v). \tag{4.2.8}$$

Of course, here the $\mathcal{E}_{nl}(v)$ are also relative to $h(r)$.

In the case of the pure polar potentials $h^{(q)}(r) = \mathrm{sgn}(q)r^q$, we obtain from (3.1.17) and (4.2.8)

$$\bar{h}_{nl}(s) = \bar{h}^{(q)}_{nl}(s) = (2/q)|q\mathcal{E}^{(q)}_{nl}/(2+q)|^{(q+2)/2}s^{-q/2}. \tag{4.2.9}$$

Now, let us suppose, for definiteness, that $pq \neq 0$ and $p > q$, so that g is strictly convex. We then have

$$\bar{h}^{(p)}_{nl}(s) > g\big(\bar{h}^{(q)}_{nl}(s)\big), \quad p > q > -2, \tag{4.2.10}$$

since, under smooth increasing transformation g, we have [8]:

$$f(r) = g\big(h(r)\big) \longrightarrow \begin{cases} \bar{f}_{nl}(s) \leq g\big(\bar{h}_{nl}(s)\big); \\ \bar{f}_{nl}(s) \geq g\big(\bar{h}_{nl}(s)\big), \end{cases} \tag{4.2.11}$$

where, $\bar{f}_{nl}(s)$ are kinetic potentials (relative to $f(r)$). We then get $\leq$ if g is concave, and $\geq$ if g is convex. If the convexity of g is strict, then the inequality in (4.2.11) is strict, $<$ or $>$. In our case,

$$\bar{f}_{nl}(s) = \bar{h}^{(p)}_{nl}(s) = (2/p)|p\mathcal{E}^{(p)}_{nl}/(2+p)|^{(p+2)/2}s^{-p/2}, \tag{4.2.12}$$

$$g\big(\bar{h}_{nl}(s)\big) = g\big(\bar{h}^{(q)}_{nl}(s)\big) = \mathrm{sgn}(p)\big(\bar{h}^{(q)}_{nl}(s)\mathrm{sgn}(q)\big)^{p/q}, \tag{4.2.13}$$

i.e.

$$g\big(\bar{h}_{nl}(s)\big) = \mathrm{sgn}(p)\big(|2/q||q\mathcal{E}^{(q)}_{nl}/(2+q)|^{(q+2)/2}s^{-q/2}\big)^{p/q}. \tag{4.2.14}$$

Now, for the case $p > q$, we have from (4.2.10) that

$$(\frac{2}{p})|p\mathcal{E}^{(p)}_{nl}/(2+p)|^{\frac{(p+2)}{2}}s^{-\frac{p}{2}} > \mathrm{sgn}(p)\big(|\frac{2}{q}||q\mathcal{E}^{(q)}_{nl}/(2+q)|^{\frac{(q+2)}{2}}s^{-\frac{q}{2}}\big)^{\frac{p}{q}}. \tag{4.2.15}$$

We first cancel the nonzero factor $s^{-\frac{p}{2}}$ from both sides, we obtain

$$(\frac{2}{p})|p\mathcal{E}^{(p)}_{nl}/(2+p)|^{(p+2)/2} > \mathrm{sgn}(p)\big(|\frac{2}{q}||q\,\mathcal{E}^{(q)}_{nl}/(2+q)|^{(q+2)/2}\big)^{\frac{p}{q}}; \tag{4.2.16}$$

then we multiply by $\mathrm{sgn}(p)$, and take the $1/p$ power of both sides of (4.2.16). Note that, in the case $p > 0$, both of these operations leave the inequality in (4.2.16) unchanged; in the case $p < 0$, the inequality is reversed twice. Hence in both cases we obtain

$$\big(|\frac{2}{p}||p\mathcal{E}^{(p)}_{nl}/(2+p)|^{(p+2)/2}\big)^{\frac{1}{p}} > \big(|\frac{2}{q}||q\mathcal{E}^{(q)}_{nl}/(2+q)|^{(q+2)/2}\big)^{\frac{1}{q}},$$

i.e.

$$|\mathcal{E}^{(p)}_{nl}|^{\frac{(2+p)}{2p}}\Big[\frac{2}{2+p}\Big]^{1/p}\Big[\frac{|p|}{2+p}\Big]^{1/2} > |\mathcal{E}^{(q)}_{nl}|^{\frac{(2+q)}{2q}}\Big[\frac{2}{2+q}\Big]^{1/q}\Big[\frac{|q|}{2+q}\Big]^{1/2}, \tag{4.2.17}$$

hence,

$$P_{nl}(p) > P_{nl}(q) > 0, \qquad pq \neq 0, \quad p > q > -2, \tag{4.2.18}$$

where, the function $P_{nl}(q)$, is as in Section III.1. Hence, the functions $P_{nl}(q)$ are strictly monotone increasing in q. Graphs of the $P_{nl}(q)$ may be found in [15]. Moreover, we have

$$P^2_{nl}(p) > P^2_{nl}(q), \quad pq \neq 0, \quad p > q > -2, \tag{4.2.19}$$

and

$$\frac{P^2_{nl}(p)}{r^2} + V(r) > \frac{P^2_{nl}(q)}{r^2} + V(r), \tag{4.2.20}$$

clearly

$$\min_{r>0} \{\frac{P^2_{nl}(p)}{r^2} + V(r)\} > \min_{r>0} \{\frac{P^2_{nl}(q)}{r^2} + V(r)\}, \tag{4.2.21}$$

i.e.

$$E^{(A)}_{nl}(p) > E^{(A)}_{nl}(q), \quad pq \neq 0, \quad p > q > -2. \tag{4.2.22}$$

Hence, the functions $E^{(A)}_{nl}(q)$ are also strictly monotone increasing in q.

Remark:

From the point of view of functional analysis [4–6] one regards the Hamiltonian operator H as a perturbation of the Laplacian $-\Delta$. Kinetic potentials are derived from the following analytical realization of this point of view [15]. We first fix $\langle -\Delta \rangle = s > 0$, this defines a certain subset D_s of the domain $\mathcal{D}_H$ of H, $H = -\Delta + v\,h(r)$. We then minimize $\langle h(r) \rangle$ over D_s, and the result, as a function of the "mean" kinetic energy s, is called the *kinetic potential* $\bar{h}_{nl}(s)$ associated with the potential shape $h(r)$. For completeness and clarity we now outline the general definition of these objects. We suppose that D_{nl} is an n-dimensional subspace of the intersection of the domain $\mathcal{D}_H$ and the angular momentum subspace of $L^2(R^3)$ labeled by the spherical harmonic $Y_l^m(\theta, \phi)$ with $m = 0$.

We now consider the union $\mathcal{D}_{nl}$ of all σ–scaled transformations, $\sigma \in R^+$ of D_{nl}, in which each wave function $\psi(\vec{r})$ in D_{nl} is replaced, by use of the rule $\psi(\vec{r}) \to \psi(\vec{r}/\sigma)$. This large union of subspaces is itself no longer a subspace; however, because $\mathcal{D}_{nl}$ contains all possible scales, we can always satisfy the constraint $(\psi, -\Delta\psi) = s$, for some $\psi \in D_{nl} \subset \mathcal{D}_{nl}$.

The idea here is that one first chooses the n-dimensional space D_{nl} and then generates the larger union $\mathcal{D}_{nl}$ of all "scaled" versions of D_{nl}.

The general definition of $\bar{h}_{nl}(s)$ is then as follows:

$$\bar{h}_{nl}(s) = \inf_{D_{nl}} \sup_{\substack{\psi \in \mathcal{D}_{nl} \\ \|\psi\|=1 \\ (\psi, -\Delta\psi)=s}} (\psi, h\psi). \tag{4.2.23}$$

IV.3 The Bounds on E_{nl}

We now study the potential

$$V(r) = ar^2 + \frac{br^2}{1+cr^2}, \quad a, b, c > 0. \tag{4.3.1}$$

The object here is to reproduce new eigenvalue bounds to E_{nl} of $H = -\Delta + V(r)$ for a wide range of potential parameters a, b and c. Our principal tool is still the "potential envelope method".

We have seen that, in the particular case of the polar "envelope basis", the method allows us to approximate the eigenvalues by means of the following semi–classical expression

$$E_{nl} \approx E_{nl}^{(A)}(q) = \min_{r>0}\left\{\left(\frac{P_{nl}(q)}{r}\right)^2 + V(r)\right\}, \tag{4.3.2}$$

where the positive numbers $P_{nl}(q)$ are determined by the eigenvalues $\mathcal{E}_{nl}^{(q)}$ of $H = -\Delta + \mathrm{sgn}(q)r^q$:

$$P_{nl}(q) = |\mathcal{E}_{nl}^{(q)}|^{(2+q)/2q}\left[\frac{2}{2+q}\right]^{1/q}\left[\frac{|q|}{2+q}\right]^{1/2}, \quad q > -2, \quad q \neq 0. \tag{4.3.3}$$

Based on a very important property that the approximations $E_{nl}^{(A)}(q)$, namely that the $E_{nl}^{(A)}(q)$ are monotonically increasing functions of q, we now study how to choose the power q of r as large as possible whilst keeping $g''(h) > 0$ for all $h > 0$, in order to obtain improved lower bounds; or as small as possible whilst keeping $g''(h) < 0$ for all $h > 0$, in order to obtain improved upper bounds. Finally we shall determine the optimal values $\{q_1, q_2\}$ of q (depending on the parameters) which guarantee respectively that $g'' > 0$ and $g'' < 0$ so

that, with these values of q, the formula (4.3.2) yields improved lower and upper energy bounds.

We therefore have to study the polar transformation function $g(h)$ defined by

$$g(t) = V(r), \quad t = h(r) = \operatorname{sgn}(q) r^q, \quad q > -2, \quad q \neq 0, \tag{4.3.4}$$

i.e.

$$g(t) = at^{2/q} + \frac{bt^{2/q}}{(1 + ct^{2/q})}. \tag{4.3.5}$$

By differentiating we find

$$g'(t) = V'(r)\frac{dr}{dt}, \quad V'(r) > 0,$$

$$dr/dt = (dt/dr)^{-1} = (q \operatorname{sgn}(q) r^{q-1})^{-1} = (|q| r^{q-1})^{-1} > 0, \tag{4.3.6}$$

hence $g'(t) > 0$, and also the following expression for the second derivative:

$$g''(t) = \frac{2b|t|^{\frac{2}{q}-2}}{q^2(1 + c|t|^{\frac{2}{q}})^3} G(s), \tag{4.3.7}$$

where

$$G(s) = 4 - s + \beta s^3, \quad s = (q+2)(1 + c|t|^{\frac{2}{q}}), \quad \beta = \frac{a(2-q)}{b(2+q)^3}. \tag{4.3.8}$$

Thus the sign of $g''(t)$ is the same as the sign of the function $G(s)$.

If $q = 2$, then $\beta = 0$, $s = 4(1 + c|t|^{\frac{2}{q}}) > 4$ and $G(s) = 4 - s < 0$. Clearly, $g'' < 0$, for all t, g is concave, therefore, $q = 2$ always yields an upper bound.

If $q < 2$, then, $\beta > 0$, for large s the sign of $G(s)$ is dominated by the term $\beta s^3 > 0$ and will eventually be positive. Thus, for $q < 2$, we do

not have $g'' < 0$ for all t and we can never obtain an upper bound. In view of the monotonicity of the approximation $E_{nl}^{(A)}(q)$ in (3.1.21), the *best* upper bound we can find this way is given by $q = 2$, which is the smallest allowed value.

We now continue to discuss the case $q < 2$. We find that

$$G'(s) = 3\beta s^2 - 1, \quad G''(s) = 6\beta s > 0, \tag{4.3.9}$$

and from the equation

$$G'(s) = 0, \quad s > (2 + q) > 0, \tag{4.3.10}$$

we get a unique critical point $\hat{s} = (3\beta)^{-1/2}$. Hence,

$$G_{min}(s) = G(\hat{s}) = 4 - \hat{s} + \beta\hat{s}^3 = 4 - \frac{2\beta^{-1/2}}{3\sqrt{3}}, \tag{4.3.11}$$

and from $G_{min}(s) \geq 0$, we have $\beta \geq 1/108$.

This after simple manipulation leads to a corresponding constraint on the parameters. We get

$$\frac{b}{a} \leq \frac{108(2-q)}{(q+2)^3}. \tag{4.3.12}$$

This important relation is illustrated in Fig.4.3(a). For those values of a and b which admit a value of q such that $g''(t) \geq 0$, we may conclude, again by the established monotonicity of $E_{nl}^{(A)}(q)$ that the best lower bound is obtained by choosing the largest such q, that is to say the value of q given by the *equality* in (4.3.12) or, equivalently, by the boundary curve shown in Fig.4.3(a).

We note that the value of $c > 0$ did not enter into these arguments. It also follows that we would obtain the same result *mutatis mutandis* for

central potentials in any number of spatial dimensions. Consequently, the bounds we have obtained are valid for all $c > 0$ and for arbitrary spatial dimension n provided only that the parameters a and b are constrained by (4.3.12).

We have taken the example $a = c = 1$, $b = 0.5$ to illustrate the sort of results we obtain. We find from (4.3.12) that the largest value of q for the best lower bound is 1.754. Meanwhile $q = 2$, the particular choice, provides the best upper bound. In Tables (1) and (2) we exhibit some results we have obtained for the *one*-dimensional and *three*-dimensional problems respectively, along with some accurate eigenvalues found by the direct numerical integration of Schrödinger equation. The latter numerical data were generated by a C++ program written by Professor R. L. Hall. In order to preserve the bounds, for the energy data quoted in these tables we obtained the $P_{nl}(q)$ values for $q = 2$ from the exact expressions

$$\begin{aligned} h(r) = r^2 \longrightarrow \mathcal{E}_{nl}^{(2)} &= v^{1/2}\,(4n + 2l - 1) \\ &\longrightarrow P_{nl}(2) = (2n + l - 1/2), \end{aligned}$$

hence

$$K_{nl}^{(h)}(r) = \Big(\frac{2n + l - 1/2}{r}\Big)^2, \tag{4.3.13}$$

and

$$h(x) = x^2 \longrightarrow P_n(2) = (n - 1/2),$$

hence

$$K_n^{(h)}(x) = (n - 1/2)^2/x^2; \tag{4.3.14}$$

the $P_{nl}(q)$ values for $q = 1.754$ were obtained by the direct numerical integration of Schrödinger's equation [15]. Since the optimal $q = 1.754$

is close to 2, the interpolation formula

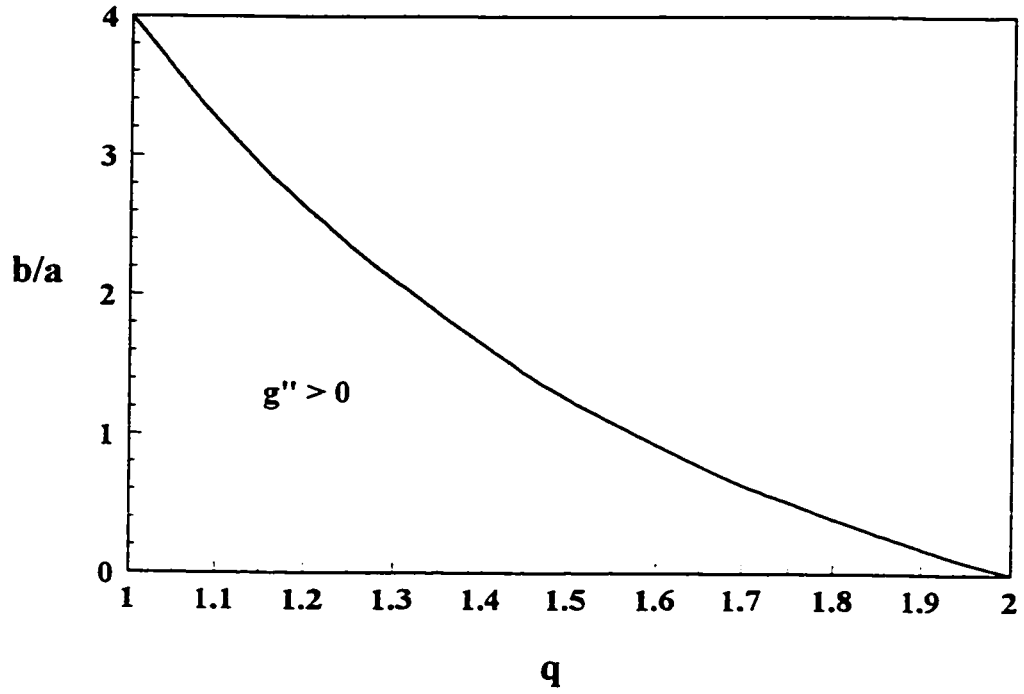
$$P_{nl}(q) = \left[(n+l)^{\alpha} + \frac{q+1}{3}[(2n+l-\frac{1}{2})^{\alpha} - (n+l)^{\alpha}]\right]^{\frac{1}{\alpha}}, \; \alpha = 3.2397, \tag{4.3.15}$$

also provides a very convenient and accurate expression for $P_{nl}(q)$, in the *three*–dimensional case.

In 1980, Hall treated the same potential in a study of the many–body problem. In this work the many–body energy was related to the energy of a specially constructed *one*–body problem ('reduced' *two*–body problem) and linear–parabolic problem envelope bounds were applied to the latter problem [1]. In the notation of the present work, the values of q employed were $q = 1$ and $q = 2$. Some cases treated in this paper correspond to the present cases: $(a = b = c = 1)$ and $(a = b = 1, c = 0.5)$. See Tables (3–6). In the earlier work, the lower bounds are weaker since only $q = 1$ was used. In the present work optimal values are chosen for q. Thus we can take $q = 1.576$ for the lower bounds. Comparing with the sequences of estimates in the caption of Fig.4.1(a), the new sequences are (3.484, 3.305, 3.507, 3.589) and (7.406, 6.918, 7.428, 7.636). The values 3.484 and 7.406 are the new values of the lower bounds for E_{10} in the two cases; in the earlier work the corresponding bounds were 3.220 and 7.053 respectively. It is readily apparent that a considerable improvement is gained for a wide range of the potential parameters.

Figure 4.3.(a)

The region beneath the boundary curve represents values of a, b, and q that satisfy the inequality (4.3.12) and guarantee that the transformation function $g(h)$ is convex. For such choices of these parameters, and any positive value of c, the semi-classical formula (3.1.21) yields energy *lower* bounds. The best lower bound is provided by the largest allowed value of q, that is to say, the value *on* the boundary curve.



CHAPTER V

TABLES

Table 1

Table of eigenvalues for the case $a = c = 1$, $b = 0.5$ in one spatial dimension. For the lower bound, the critical value of q is $q = 1.754$; for the upper bound, $q = 2$. E_n^L and E_n^U are the lower and upper bounds obtained from (3.1.21), and E_n is an accurate approximation obtained by the direct numerical integration of Schrödinger's equation.

n	E_n^L	E_n	E_n^U
1	1.109	1.119	1.161
2	3.239	3.256	3.298
3	5.251	5.295	5.356
4	7.249	7.324	7.388
5	9.228	9.342	9.409
6	11.205	11.356	11.423
7	13.175	13.367	13.433
8	15.145	15.375	15.441
9	17.113	17.382	17.447
10	19.088	19.388	19.452
11	21.080	21.394	21.456

Table 2

Table of eigenvalues for the case $a = c = 1$, $b = 0.5$ in three spatial dimension. For the lower bound, the critical value of q is $q = 1.754$; for the upper bound, $q = 2$. $E^L_{n\ell}$ and $E^U_{n\ell}$ are the lower and upper bounds obtained from (3.1.21), and $E_{n\ell}$ is an accurate approximation obtained by the direct numerical integration of Schrödinger's equation.

n	ℓ	$E^L_{n\ell}$	$E_{n\ell}$	$E^U_{n\ell}$
1	0	3.239	3.256	3.298
2	0	7.249	7.324	7.388
3	0	11.205	11.356	11.423
4	0	15.145	15.375	15.441
1	1	5.296	5.327	5.356
2	1	9.255	9.357	9.409
3	1	13.195	13.376	13.433
4	1	17.128	17.389	17.447
1	2	7.328	7.368	7.388
2	2	11.262	11.383	11.423
3	2	15.190	15.394	15.441
4	2	19.123	19.403	19.452
1	3	9.348	9.394	9.409
2	3	13.267	13.403	13.433
3	3	17.188	17.409	17.447
4	3	21.135	21.415	21.456

Table 3

Table of eigenvalues for the case $a = b = c = 1$ in one spatial dimension. For the lower bound, the critical value of q is $q = 1.576$; for the upper bound, $q = 2$. E_n^L and E_n^U are the lower and upper bounds obtained from (3.1.21), and E_n is an accurate approximation obtained by the direct numerical integration of Schrödinger's equation.

n	E_n^L	E_n	E_n^U
1	1.211	1.232	1.310
2	3.484	3.507	3.590
3	5.518	5.589	5.710
4	7.526	7.648	7.775
5	9.492	9.684	9.816
6	11.456	11.712	11.845
7	13.406	13.733	13.866
8	15.362	15.750	15.881
9	17.333	17.764	17.894
10	19.362	19.777	19.904
11	21.498	21.788	21.912

Table 4

Table of eigenvalues for the case $a = b = c = 1$ in three spatial dimension. For the lower bound, the critical value of q is $q = 1.576$; for the upper bound, $q = 2$. $E^L_{n\ell}$ and $E^U_{n\ell}$ are the lower and upper bounds obtained from (3.1.21), and $E_{n\ell}$ is an accurate approximation obtained by the direct numerical integration of Schrödinger's equation.

n	ℓ	$E^L_{n\ell}$	$E_{n\ell}$	$E^U_{n\ell}$
1	0	3.484	3.507	3.589
2	0	7.526	7.648	7.775
3	0	11.456	11.712	11.845
4	0	15.362	15.750	15.881
1	1	5.603	5.651	5.710
2	1	9.544	9.713	9.816
3	1	13.444	13.751	13.866
4	1	17.361	17.777	17.894
1	2	7.669	7.734	7.775
2	2	11.561	11.765	11.845
3	2	15.444	15.787	15.881
4	2	19.417	19.804	19.904
1	3	9.710	9.787	9.816
2	3	13.574	13.804	13.866
3	3	17.562	17.818	17.894
4	3	21.559	21.829	21.913

Table 5

Table of eigenvalues for the case $a = b = 1$, $c = 0.5$ in one spatial dimension. For the lower bound, the critical value of q is $q = 1.576$; for the upper bound, $q = 2$. E_n^L and E_n^U are the lower and upper bounds obtained from (3.1.21), and E_n is an accurate approximation obtained by the direct numerical integration of Schrödinger's equation.

n	E_n^L	E_n	E_n^U
1	1.251	1.293	1.357
2	3.703	3.714	3.818
3	5.883	5.921	6.086
4	7.996	8.053	8.257
5	10.038	10.145	10.374
6	12.059	12.215	12.459
7	14.052	14.270	14.524
8	16.037	16.314	16.575
9	18.007	18.352	18.616
10	19.973	20.383	20.650
11	21.930	22.411	22.678

Table 6

Table of eigenvalues for the case $a = b = 1$, $c = 0.5$ in three spatial dimension. For the lower bound, the critical value of q is $q = 1.576$; for the upper bound, $q = 2$. $E^L_{n\ell}$ and $E^U_{n\ell}$ are the lower and upper bounds obtained from (3.1.21), and $E_{n\ell}$ is an accurate approximation obtained by the direct numerical integration of Schrödinger's equation.

n	ℓ	$E^L_{n\ell}$	$E_{n\ell}$	$E^U_{n\ell}$
1	0	3.703	3.713	3.818
2	0	7.996	8.052	8.257
3	0	12.060	12.214	12.459
4	0	16.047	16.314	16.575
1	1	5.973	5.988	6.086
2	1	10.093	10.180	10.374
3	1	14.093	14.291	14.524
4	1	18.076	18.367	18.616
1	2	8.146	8.175	8.257
2	2	12.168	12.289	12.459
3	2	16.130	16.366	16.575
4	2	20.157	20.422	20.649
1	3	10.264	10.308	10.374
2	3	14.227	14.379	14.524
3	3	18.178	18.432	18.616
4	3	22.321	22.474	22.678

CHAPTER VI

CONCLUSION

Over seventeen years have past since the potential envelope method was originally introduced by Hall [1]. The method is still full of vitality. The derivation of the method was based on the Min–Max Principle and the Comparison Theorem; it's success is a consequence of its simplicity and generality.

How do Schrödinger eigenvalues depend on parameters in the potential? The envelope approximation was designed to try to answer this question by providing simple general formulas derived from a semiclassical approximation in which the potential, along with its parameters, appears explicitly. Most of the analytical effort involved in an application is directed towards the issue of convexity which provides sufficient conditions guaranteeing that the approximations are also energy *bounds*.

It is an interesting feature of the present work that the bound conditions are not dependent on the number of spatial dimensions. Once these conditions have been determined, it is easy to obtain the approximations from the simple general expression (3.1.21)

$$E_{nl} \approx E_{nl}^{(A)}(q) = \min_{r>0}\left\{\left(\frac{P_{nl}(q)}{r}\right)^2 + V(r)\right\},$$

where

$$V(r) = g(h(r)), \quad h(r) = \mathrm{sgn}(q)r^q,$$

and g has definite convexity,

$$\approx = \leq \qquad \text{if } g \text{ is concave,}$$

$$\approx = \geq \qquad \text{if } g \text{ is convex.}$$

Such formulas are easily accommodated by a microcomputer. The simplicity of the approach would enable other aspects of the spectral inheritance of the form of the potential to be explored. Such investigations, however, are not immediately facilitated by an abundance of purely numerical data.

On the other hand, we have seen that in the special procedure using the simple pure polar transformation function defined by

$$g(h) = V(r),\ h(r) = \mathrm{sgn}(q)r^q, \quad q > -2, \quad q \neq 0,$$

there is a clear way to improve the energy bounds. We can choose the power q of r as large as possible whilst keeping $g''(h) > 0$ for all $h > 0$, in order to obtain improved lower bounds; or as small as possible whilst keeping $g''(h) < 0$ for all $h > 0$, in order to obtain improved upper bounds. In the present work, the numerical results obtained for a wide range of potential parameters demonstrate the marked improvement of the bounds which is obtainable by optimization with respect to q. These numerical results are presented in Tables 1–6.

REFERENCES

1. R. L. Hall, *Phys. Rev.* **D22**, 2062 (1980).
2. A. Weinstein and W. Stenger, *Method of Intermediate Problems for Eigenvalues* (Academic, New York, 1972).
3. R. L. Hall, *J. Phys. A: Math. Gen.* **25** (1992)
4. M. Reed and B. Simon, *Method of Modern Mathematical Physics IV: Analysis of Operators* (Academic, New York, 1972).
5. E. Prugovečki, *Quantum Mechanics in Hilbert Space* (Academic, New York, 1972).
6. W. Thirring, *A Course in Mathematical Physics 3: Quantum Mechanics of Automs and Molecules* (Springer, New York, 1981).
7. B. Epstein, *Linear Functional Analysis: An Introduction to Lebesgue Integration and Infinite Dimensional Problems* (W. B. Saunders, London, 1970).
8. I. M. Gelfand and S. V. Fomin, *Calculus of Variations* (Prentice–Hall, Englewood Cliffs, NJ, 1963)
9. R. L. Hall, *Phys. Rev. D:Part.Fields* **23**,1421 (1981).
10. R. L. Hall, *J. Math. Phys.* **24**, 324 (1983).
11. R. L. Hall, *J. Math. Phys.* **25**, 2708 (1984)

12. J. P. Duarte and R. L. Hall, *Can. J. Phys.* **69**, 1362 (1991).

13. R. L. Hall, *J. Phys. A:Math.Gen.* **25**, 4459 (1992).

14. R. L. Hall, *J. Math. Phys.* **34**, 2779 (1993).

15. R. L. Hall, *Phys. Rev.* **A39**, 5500 (1989).

16. A. K. Mitra, *J. Math. Phys.* **19**, 2018 (1978).

17. S. Galicia and J. P. Killingbeck, *Phys. Lett.* **71A**, 17 (1979).

18. R. S. Kaushal, *J. Phys. A: Math. Gen.* **12**, L253 (1979).

19. N. Bessis and G. Bessis, *J. Math. Phys.* **21**, 2780 (1980).

20. G. P. Flessas, *Phys. Lett.* **83A**,121 (1981).

21. K. V. Bhagwat, *J. Phys.A: Math.Gen.* **14**,377 (1981).

22. V. S. Varma, *J. Phys. A: Math. Gen.* **14**, L489 (1981).

23. C. S. Lai and H. E. Lin, *J. Phys. A: Math. Gen.*, **15**,1495 (1982).

24. C. R. Handy, *J. Phys. A: Math. Gen.* **18**, 3593 (1985).

25. V. Fack and G. V. Berghe, *J. Phys. A: Math. Gen.* **18**, 3355 (1985).

26. M. H. Blecher and P. G. L. Leach, *J. Phys.A: Math.Gen.* **20**, 5923 (1987).

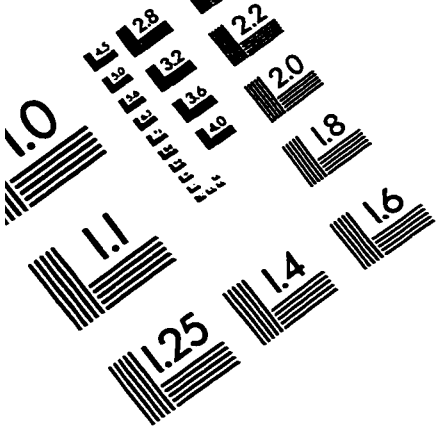
27. R. J. W. Hodgson, *J. Phys. A: Math. Gen.* **21**, 1563 (1988).

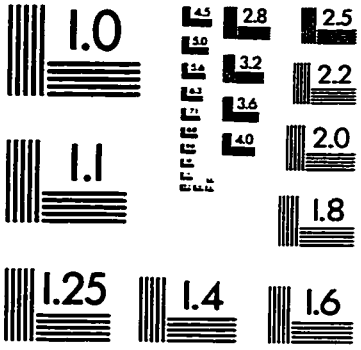
28. M. Znojil, *J. Phys. A: Math. Gen.* **16**, 293 (1983).

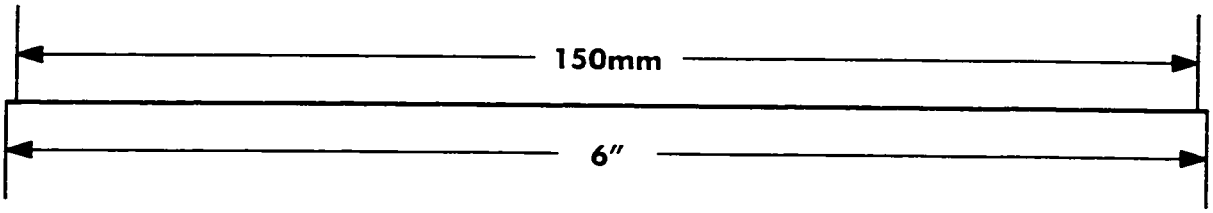
29. B. Roy, R. Roychoudhury and P. Roy, *J. Phys. A: Math. Gen.* **21**, 1579 (1988).

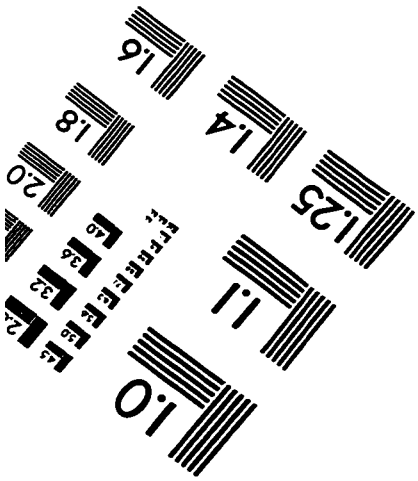
30. M. R. M. Witwit, *J. Phys. A: Math. Gen.* **24**, 5291 (1991).

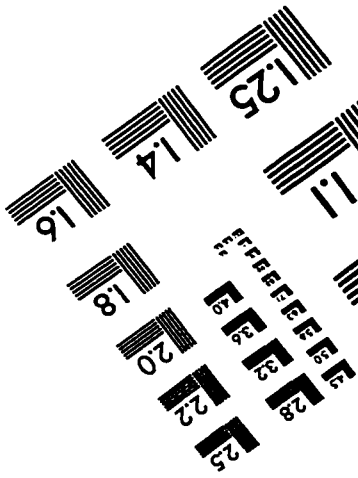
31. C. R. Handy, *J. Phys. A: Math. Gen.* **26**, 2653 (1993).











APPLIED IMAGE, Inc
1653 East Main Street
Rochester, NY 14609 USA
Phone: 716/482-0300
Fax: 716/288-5989